

Gauge invariant grid discretization of Schrödinger equation

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Using the Wilson formulation of lattice gauge theories, a gauge invariant grid discretization of a one-particle Hamiltonian in the presence of an external electromagnetic field is proposed. This Hamiltonian is compared both with that obtained by a straightforward discretization of the continuous Hamiltonian by means of balanced difference methods, and with a tight-binding Hamiltonian. The proposed Hamiltonian and the balanced difference one are used to compute the energy spectrum of a charged particle in a two-dimensional parabolic potential in the presence of a perpendicular, constant magnetic field. With this example we point out how a “naïve” discretization gives rise to an explicit breaking of the gauge invariance and to large errors in the computed eigenvalues and corresponding probability densities; in particular, the error on the eigenfunctions may lead to very poor estimates of the mean values of some relevant physical quantities on the corresponding states. On the contrary, the proposed discretized Hamiltonian allows a reliable computation of both the energy spectrum and the probability densities.

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I. INTRODUCTION

In the last few years, there has been increasing activity concerning numerical simulations of low energy quantum systems and in this context particular attention has been paid to mesoscopic systems such as low-dimensional semiconductor nanostructures. Of special interest are “quasi zero” dimensional systems; in this case, the electrons are confined in a small region of space—as in an atom—and hence they exhibit a quantized energy spectrum. In particular, urged by many experimental results¹, theoretical investigations of the influence of a magnetic field on the spectrum of such systems of confined electrons have been carried out².

The problem of computing the energy spectrum of such systems has been addressed in many ways^{3–8}. In most of the approaches used the resulting Schrödinger equation is solved numerically, introducing a discretization grid and using finite difference methods (see e.g.⁸). In order to study the effect due to the presence of a magnetic field, the common procedure is to introduce a vector potential (“gauge field”) and eventually construct an appropriate discretization of the corresponding Hamiltonian. On the other hand, it is well known from lattice quantum field theory that the presence of a gauge field may lead to the breaking of the gauge invariance if the Hamiltonian is naively discretized on a grid. In particular the eigenvalues of the Hamiltonian and the probability density associated with a given eigenfunction (i.e. its square modulus) could depend on the gauge choice.

The aim of this paper is to present a method of constructing a grid-discretized one-particle Hamiltonian in the presence of an external electromagnetic field, that leads to a manifest gauge invariance of the mean values of the observables on its eigenstates. In order to do so we apply the Wilson formulation of lattice gauge theories⁹ (for a review on this topic see also¹⁰).

The paper is organized as follows: in Sec. II, we construct explicitly a lattice discretization of the one particle Hamiltonian in the presence of an external electromagnetic field using the above mentioned formulation and we compare it with that obtained by introducing directly the vector potential and with a tight-binding one. In particular, we write the proposed Hamiltonian in the tight-binding formalism and we show that it leads to a simpler expression for the hopping potential. In Sec. III we use the “naïve” discretized Hamiltonian and the gauge-invariant one to compute the energy spectrum of a charged particle in a two-dimensional parabolic potential in the presence of a perpendicular, constant magnetic field, showing explicitly that the Wilson formulation preserves the gauge invariance. Finally, Sec. IV contains some concluding remarks.

II. GAUGE INVARIANT LATTICE HAMILTONIAN

In this section we apply the Wilson formulation to find a Hamiltonian H_{LATT} defined on a lattice of discretization points that in the continuum limit (i.e. lattice spacing going to zero) tends to the following generic Hamiltonian

operator for a particle with charge q in the presence of a magnetic field $\vec{B}(\vec{r}) = \vec{\nabla} \wedge \vec{A}(\vec{r})$ and of an electrostatic potential $V(\vec{r})$:

$$H_{\text{CONT}} = \frac{\hbar^2}{2m} \left[-\nabla^2 + ig \left\{ \vec{A}(\vec{r}), \vec{\nabla} \right\} + g^2 \left| \vec{A}(\vec{r}) \right|^2 \right] + V(\vec{r}), \quad (1)$$

where $g = q/\hbar$, and the symbol $\{\vec{A}(\vec{r}), \vec{\nabla}\}$ stands for the sum of the anticommutators for the components of \vec{A} and $\vec{\nabla}$. Throughout this paper, for simplicity we neglect the spin.

The essential requirement we impose is that the lattice Hamiltonian H_{LATT} maintains all the properties of the continuum one for a gauge transformation of the vector potential.

It is well known from elementary quantum mechanics that when the vector potential transforms as

$$\vec{A} \rightarrow \vec{A} + \vec{\nabla} \Lambda(\vec{r}) \quad (2)$$

a generic wave function $\Psi(\vec{r})$, corresponding to a physical state of the system, transforms as

$$\Psi(\vec{r}) \rightarrow G(\vec{r}) \Psi(\vec{r}), \quad \text{with} \quad G(\vec{r}) = \exp\{ig\Lambda(\vec{r})\}, \quad (3)$$

leaving unchanged the mean values of the observables on Ψ . In the following, we shall refer to the above mentioned property as gauge invariance. More formally, under the gauge transformation (2) the Hamiltonian H_{CONT} behaves as

$$H_{\text{CONT}} \rightarrow G(\vec{r}) H_{\text{CONT}} G^\dagger(\vec{r}), \quad (4)$$

and, as a wave function Ψ transforms according to (3), the energy functional

$$\mathcal{E}_c[\Psi] = \int d\vec{r} \Psi^\dagger(\vec{r}) H_{\text{CONT}} \Psi(\vec{r}) \quad (5)$$

is left unchanged.

We now introduce a uniform discretization grid with lattice constant a , such that a generic point on it is identified with a vector $x = (la, ma, na)$; we shall also indicate a generic direction in the discretized space with the Greek letter μ . Given a vector potential with components $A_\mu(x)$, following⁹ we define on the lattice the operators $U_\mu(x)$ as follows:

$$U_\mu(x) = \exp\{iga A_\mu(x)\}. \quad (6)$$

Let us consider the discrete gauge transformation corresponding to (2), i.e.

$$A_\mu \rightarrow A_\mu + \frac{1}{a} [\Lambda(x + \mu) - \Lambda(x)], \quad (7)$$

where $x + \mu$ denotes the next neighbor of x in the μ direction. It is straightforward to show that under gauge transformations (7) U_μ behaves as

$$U_\mu(x) \rightarrow G^\dagger(x) U_\mu(x) G(x + \mu), \quad \text{with} \quad G(x) = \exp\{ig\Lambda(x)\}. \quad (8)$$

In the following, we represent the discretized Hamiltonian operator \hat{H}_{LATT} with its matrix elements between the functions $\chi(x - x_i) = 1/\sqrt{a^3} \delta_{x, x_i}$, where δ_{x, x_i} is equal to zero anywhere on the grid except at the lattice point x_i where it equals 1, and $1/\sqrt{a^3}$ is a normalization factor. Hence we define $H_{\text{LATT}}(x, y)$ as:

$$H_{\text{LATT}}(x, y) = a^3 \sum_{\bar{x}} \chi^\dagger(\bar{x} - x) \hat{H}_{\text{LATT}} \chi(\bar{x} - y) = \sum_{\bar{x}} \delta_{\bar{x}, x} \hat{H}_{\text{LATT}} \delta_{\bar{x}, y}. \quad (9)$$

With the definition above we have:

$$\hat{H}_{\text{LATT}} \Psi(x) = \sum_y H_{\text{LATT}}(x, y) \Psi(y). \quad (10)$$

We now want to construct a lattice Hamiltonian which transforms as

$$H_{\text{LATT}}(x, y) \rightarrow G(x) H_{\text{LATT}}(x, y) G^\dagger(y). \quad (11)$$

As in the continuum case, this implies that a wave function $\Psi(\vec{r})$ transforms according to the discrete analog of (3):

$$\Psi(x) \rightarrow G(x)\Psi(x). \quad (12)$$

We find that the following Hamiltonian

$$H_{\text{WH}}(x, y) = \frac{\hbar^2}{2m} \sum_{\mu} \frac{1}{a^2} [2\delta_{x,y} - U_{\mu}(y) \delta_{x-\mu,y} - U_{\mu}^{\dagger}(x) \delta_{x+\mu,y}] + V(x)\delta_{x,y} \quad (13)$$

has the correct continuum limit (1) and it transforms as required by Eq. (11). Moreover the Hamiltonian (13) gives rise, as in the continuum case, to a gauge invariant energy functional

$$\mathcal{E}_{\text{LATT}}[\Psi] = a^3 \sum_{x,y} \Psi^{\dagger}(x) H_{\text{WH}}(x, y) \Psi(y). \quad (14)$$

In order to show the advantages of the above formulation in respect to a straightforward discretization of (1) we now consider the discrete Hamiltonian obtained from (1) applying balanced difference methods, which reads:

$$H_{\text{BDH}}(x, y) = \frac{\hbar^2}{2m} \sum_{\mu} \frac{1}{a^2} \left\{ \left[2 + \frac{iga}{2} (A_{\mu}(x+\mu) - A_{\mu}(x-\mu)) + g^2 a^2 A_{\mu}^2(x) \right] \delta_{x,y} - (1 + iga A_{\mu}(x)) \delta_{x-\mu,y} - (1 - iga A_{\mu}(x)) \delta_{x+\mu,y} \right\} + V(x)\delta_{x,y}. \quad (15)$$

One of the inconveniences of the Hamiltonian (15) is that it is not Hermitian and becomes such only in the continuum limit.

As a discretized Hamiltonian is generally used to compute the lowest bound states of a system, we discuss briefly the error introduced by the discretization in this kind of computation. In particular we focus our attention on the error made when a discretized Hamiltonian acts on the eigenfunctions corresponding to the bound states we wish to compute. For this purpose we consider the quantity:

$$\Delta_n(x) = \left| \Psi_n^{\dagger}(x) H_{\text{CONT}}(x) \Psi_n(x) - \sum_y \Psi_n^{\dagger}(x) H_{\text{LATT}}(x, y) \Psi_n(y) \right|, \quad (16)$$

where Ψ_n is the exact wave function corresponding to the n -th eigenvalue of H_{CONT} and all quantities are evaluated at a generic grid point x . It is worth noticing that the error Δ_n has a component due to the discretization of the Laplacian operator on the grid and an other due to the discretization of the gauge field. The systematic error due to the discretization of the spatial derivatives is

$$\Delta_n^0(x) = \frac{1}{6} \left| \Psi_n^{\dagger}(x) \sum_{\mu} \frac{\partial^4 \Psi_n}{\partial x_{\mu}^4} \right|_x \frac{\hbar^2}{2m^*} a^2. \quad (17)$$

This error is the same for both Hamiltonians (13) and (15). As far as it concerns the error due to the discretization of the gauge field, the following considerations apply: When in Eq. (16) for H_{LATT} we use H_{WH} (given by Eq. 13), both $\Psi_n^{\dagger}(x) H_{\text{CONT}}(x) \Psi_n(x)$ and $\sum_y \Psi_n^{\dagger}(x) H_{\text{WH}}(x, y) \Psi(y)$ are gauge invariant; hence the contribution to Δ_n due to the vector potential is gauge invariant too and it depends only upon the coupling between the particle and the field (i.e. g), upon the magnetic field \vec{B} and upon the lattice spacing a . It may be shown that the component of the error Δ_n due to the vector potential is small for any lattice point x if:

$$|ga^2 \vec{B}(x)| \ll 1 \quad \forall x. \quad (18)$$

Therefore, when condition (18) is satisfied and the systematic error (17) is small for the states we wish to compute, the Hamiltonian (13) is a good approximation of (1). We notice that Eq. (18) is consistent with the fact that the stronger the magnetic field the more localized are the eigenfunctions and thus a smaller lattice spacing a is required to get a good description of them. Instead, if in Eq. (18) we use H_{BDH} , then the quantity $\sum_y \Psi^{\dagger}(x) H_{\text{BDH}}(x, y) \Psi(y)$ is no more gauge invariant and as a consequence the error Δ_n depends on the choice of the vector potential \vec{A} . In particular for some “unhappy” gauge choices the error given by (16) may be so large that (15) becomes useless even for a rough estimate of the ground state energy.

As tight-binding Hamiltonians are often used to discretize the Schrödinger equation on a lattice, it is interesting to see how the proposed Hamiltonian (13) compares to them. Without a magnetic field, a tight binding Hamiltonian (see e.g.¹¹) is equivalent to that obtained with balanced difference methods, although written with another formalism. In the presence of a gauge field, a phase shift is introduced in the hopping potential¹². A tight-binding Hamiltonian, for discretizing a Schrödinger problem in the presence of a magnetic field, reads:

$$H_{\text{TB}} = \sum_x \left[N_d \frac{\hbar^2}{ma^2} + V(x) \right] |x\rangle\langle x| + \sum_x \sum_{y \neq x} \left(-\frac{\hbar^2}{2ma^2} \right) e^{i\theta_{x,y}} |x\rangle\langle y|, \quad (19)$$

where N_d is the number of dimensions, the summation over y extends only to the next-neighbor of the lattice point x , and the phase shift is given by:

$$\theta_{x,y} = -\frac{q}{\hbar} \int_x^y \vec{A} \cdot d\vec{\mu}, \quad (20)$$

with the integration being performed on the straight line connecting the two points x and y . The first thing to notice is that Hamiltonian (19) has the correct continuum limit and is gauge invariant, as can be easily proved. The expression (20) for the phase shift was introduced for the tight-binding computation of electronic states in crystal lattices. For a crystal, the lattice constant is fixed and depends on the particular structure being investigated; therefore the gauge field \vec{A} can vary considerably over a lattice constant and thus the use of an integral in the phase shift (20) is needed. This consideration does not apply to the case of a lattice of discretization points, as the lattice constant is chosen sufficiently small in order to get a good approximation. We also wish to point out that the proposed Hamiltonian (13) can be written in the tight-binding formalism:

$$H_{\text{TBW}} = \sum_x \left[N_d \frac{\hbar^2}{2ma^2} + V(x) \right] |x\rangle\langle x| + \sum_{x,\mu} \left(-\frac{\hbar^2}{2ma^2} \right) \left[U_\mu(x-\mu) |x\rangle\langle x-\mu| + U_\mu^\dagger(x) |x\rangle\langle x+\mu| \right]. \quad (21)$$

Equation (21) suggests a simpler expression for the hopping potential in the presence of a magnetic field. In fact the magnetic field can be taken into account by introducing the lattice operator U_μ . Moreover, the Hamiltonian (21) does not require the knowledge of the gauge field over the entire space but just on the lattice points; this is very useful if the vector potential is computed by some discretization technique. Finally, it is worth noticing that, as far as the discretization of a Schrödinger problem is concerned, Hamiltonian (21) is practically coincident with (19), although Eq. (19) is more complicated.

III. NUMERICAL EXAMPLE

In this section, we use Hamiltonians (13) and (15) to compute the lowest part of the energy spectrum and the corresponding eigenfunctions for an exactly solvable problem: an electron confined in a two-dimensional parabolic potential in GaAs in the presence of a constant perpendicular magnetic field of strength B . The fact that this problem is analytically solvable allows us to test the accuracy of the discretized Hamiltonians and their behavior under gauge transformations.

The Hamiltonian of the system is:

$$H_{\text{CONT}} = \frac{\hbar^2}{2m^*} \left[-\nabla^2 + ig \left\{ \vec{A}(\vec{r}), \vec{\nabla} \right\} + g^2 \left| \vec{A}(\vec{r}) \right|^2 \right] + \frac{1}{2} m^* \Omega^2 |\vec{r} - \vec{r}_C|^2, \quad (22)$$

where $g = -e/\hbar$ with e modulus of the electron charge, $\hbar\Omega$ is the confining energy, \vec{r}_C is the coordinate of the center of the parabolic potential, and m^* is the effective mass for an electron in GaAs.

To approach analytically the problem of computing the eigenvalues and the eigenvectors of the Hamiltonian (22), it is convenient to use spherical coordinates on the plane where the electron is confined with the origin at the center of the parabolic potential.

With the gauge choice $\vec{A} = -(1/2)\vec{r} \wedge \vec{B}$, the eigenvalues and eigenvectors of (22) are given by¹³:

$$E_{n,M} = \frac{1}{2} \hbar \Omega_{eff} (2n + |M| + 1) + \frac{1}{2} \hbar \omega_c M \quad (23)$$

$$\Psi_{n,M} = \frac{1}{\lambda \sqrt{2\pi}} \sqrt{\frac{n!}{(n+|M|)!}} e^{iM\varphi} \exp\left(-\frac{r^2}{4\lambda^2}\right) \left(\frac{r^2}{2\lambda^2}\right)^{\frac{|M|}{2}} L_n^{|M|} \left(\frac{r^2}{2\lambda^2}\right), \quad (24)$$

where $\omega_c = eB/m^*$, $\Omega_{eff}^2 = 4\Omega^2 + \omega_c^2$, $\lambda^2 = \hbar/(m^*\Omega_{eff})$, n is a non negative integer quantum number, M is the angular momentum quantum number and $L_n^{[M]}$ is the n -th Laguerre polynomial.

In order to compute numerically the lowest eigenvalues and eigenvectors of (22) with the discretized Hamiltonians (13) and (15), we introduce a finite square grid centered around the point \vec{r}_C , and we impose Dirichlet boundary conditions. This is equivalent to approximating the parabolic potential V with a potential \tilde{V} which is equal to V inside the grid region and goes to infinity outside it. We notice that the larger the region covered by the grid the more eigenvalues of (22) can be effectively approximated. In the following part of this section, dealing with the discretized computation, we use an orthogonal coordinate system with the grid placed in the first quadrant of the xy plane and the z -axis perpendicular to it. In all the numerical simulations we have taken a confining energy $\hbar\Omega$ of 4 meV and we have used for m^* the value $0.067m_0$ with m_0 being the electron mass. We have used a grid of 99×99 points and a lattice constant a of 2.4 nm, thus covering a region of 240 nm \times 240 nm.

As our purpose is to investigate the behavior of the discretized Hamiltonians (13) and (15) under gauge transformations, we compute the eigenvalues and the eigenvectors for the following three gauge choices:

$$\begin{aligned} \text{gauge 1:} \quad A_x &= -\frac{y}{2} B \\ A_y &= \frac{x}{2} B \end{aligned} \tag{25}$$

$$\begin{aligned} \text{gauge 2:} \quad A_x &= -\frac{y - y_C}{2} B \\ A_y &= \frac{x - x_C}{2} B \end{aligned} \tag{26}$$

$$\begin{aligned} \text{gauge 3:} \quad A_x &= -(x - y) B \\ A_y &= y B. \end{aligned} \tag{27}$$

These gauges are transverse; in particular, gauge 1 corresponds to $\vec{A} = -(1/2)\vec{r} \wedge \vec{B}$, while gauge 2 corresponds to $\vec{A} = -(1/2)(\vec{r} - \vec{r}_C) \wedge \vec{B}$. Gauge 2 is similar to gauge 1, but symmetric with respect to the center of parabolic potential and, as we shall see below, it yields more accurate results with respect to the other two gauges when inserted in the naively discretized Hamiltonian (15). In the following, we shall refer to the Hamiltonians (13) and (15) as WH (Wilson Hamiltonian) and BDH (Balanced Difference Hamiltonian) respectively.

In Fig. 1 we show the lowest fifteen eigenenergies for a magnetic field strength of 10 T, computed with WH and BDH, together with the exact ones. We have numbered the eigenvalues with an integer i so that $E_i \leq E_{i+1}$ and we plot them versus i . We have found that the results obtained using WH with the three gauges (25,26,27) do not differ; therefore for the quantities computed with WH we do not specify which gauge we have used. From the above mentioned figure, we notice that: (1) The eigenvalues computed with BDH using gauges 1 and 3 differ appreciably from the exact ones; in particular, this difference grows with increasing eigenvalue. (2) The eigenvalues computed with BDH using gauge 2 tend to differ from the exact ones for the excited states.

The explicit breaking of gauge invariance present in the Hamiltonian can be further investigated analyzing the probability density $|\Psi_{n,M}|^2$: in Fig. 2 we show the probability density for the ground state (with $B = 10$ T) using either the corresponding exact eigenfunction (from Eq. 24) or that obtained with BDH; for this computation we have not found significant differences between the exact probability density and either that computed with WH (using the three different gauges) or that computed with BDH using gauge 2. From Fig 2 it is evident that in this case the breaking of gauge-invariance of BDH “disrupts” the symmetry of the probability density with respect to the center of the confining potential. We have found the same phenomenon with the gauge 3, while this does not occur using gauge 2 because this gauge preserves the above mentioned symmetry.

In Fig. 3 we report the probability density for the 14-th excited state, i.e. that with $n = 0, M = -14$ (see Eq. 23), and $B = 10$ T using the corresponding exact eigenfunction and that computed with BDH using gauge 2; also in this case we have not found significant differences between the exact calculation and the one performed with WH, while it is evident that the result obtained with BDH using gauge 2 does not match the exact one. At this point it is worth stressing that even if in some cases, for a careful gauge choice, BDH gives a good estimate of the eigenenergies, the estimate of the corresponding wave functions may be inadequate (see Fig 1 and Fig. 3). This implies that the matrix elements of an operator corresponding to an observable physical quantity (e.g. dipole and quadrupole momenta) between the eigenfunctions computed with BDH can be affected by large errors.

Finally, in Fig. 4 we show the ground state energy as a function of the magnetic field magnitude computed with the exact expression and with the three different gauges using both WH and BDH. The results obtained using WH with the three gauges (25,26,27) do not differ; therefore for the quantities computed with WH the gauge used is not specified. This analysis shows how the effect of the breaking of the gauge invariance in the spectrum of BDH grows with increasing magnetic field magnitude.

IV. CONCLUSIONS

In this paper we have addressed the problem of developing a method to find a gauge invariant grid discretization of a one-particle Hamiltonian in the presence of an external electromagnetic field; for this purpose, we have used the Wilson formulation of lattice gauge theories. This Hamiltonian, written in the tight-binding formalism, leads to a simpler expression for the hopping potential, that does not require the knowledge of the gauge field over the entire space but only on the lattice of discretization points. The method developed has been checked in an exact solvable case, i.e. a Hamiltonian describing an electron confined in a two-dimensional parabolic potential in the presence of a constant perpendicular magnetic field. The results obtained clearly show how a “naïve” discretization yields to an explicit breaking of the gauge invariance and may lead to large errors in the estimates of the eigenvalues and corresponding probability densities. With a careful gauge choice a naively discretized Hamiltonian can be used to give a rough estimate of the energy spectrum, but the corresponding eigenfunctions are still affected by large errors, thus being unsuitable for the computation of the matrix elements of operators corresponding to relevant physical quantities. On the other hand, the proposed discretized Hamiltonian (13) has the correct behavior under gauge transformations and allows an accurate computation of both the energy spectrum and the probability densities.

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- ¹ W. Hansen *et al.* Phys. Rev. Lett. **62**, 2168 (1989);
T. Demel, D. Heitmann, P. Granbow, and K. Ploog, Phys. Rev. Lett. **64**, 788 (1990)
- ² A. Kumar, S. E. Laux, F. Stern, Phys. Rev. B **42**, 5166 (1990).
- ³ G. W. Bryant, Phys. Rev. Lett. **59**, 1140 (1987).
- ⁴ B. L. Johnson, G Kirczenow, Phys. Rev. B **47**, 10563 (1993).
- ⁵ M. Stopa, Phys. Rev. B **48**, 18340 (1993).
- ⁶ M. Macucci, K. Hess, G. J. Iafrate, J. Appl. Phys. **77**, 3267 (1995).
- ⁷ M. Stopa, Phys. Rev. B **54**, 13767 (1996).
- ⁸ M. Macucci, K. Hess, G. J. Iafrate, Phys. Rev. B **55**, 4879 (1997).
- ⁹ K. Wilson, Phys. Rev. **D 10**, 2445 (1974).
- ¹⁰ K. Wilson, in *New phenomena in Subnuclear Physics*, edited by A. Zichichi (1977).
J.B. Kogut, “*From asymptotic freedom to fermion computer simulations: Lectures in lattice gauge theory*”, proceedings of the International School “Enrico Fermi”, Varenna, edited by N. Cabibbo (1984), p. 315-388 *and references therein*.
- ¹¹ F. Sols, M. Macucci, U. Ravaioli, and K. Hess, J. Appl. Phys. **66**, 3892 (1989).
- ¹² G. Y. Oh, M. H. Lee, Phys. Rev. **B 53**, 1225 (1996).
- ¹³ V. Fock, Z. Phys. **47**, 446 (1928).

FIG. 1. Lowest fifteen eigenvalues for $B = 10\text{T}$ computed with: exact Hamiltonian (points); WH (diamonds); BDH with gauge 1 (circles); BDH with gauge 2 (cross); BDH with gauge 3 (squares).

FIG. 2. Ground state probability density for $B = 10\text{T}$: a) exact; b) computed with BDH (gauge 1).

FIG. 3. Probability density of the 14-th excited state ($n = 0$, $M = -14$): a) exact; b) computed with BDH (gauge 2).

FIG. 4. Ground state energy plotted against magnetic field magnitude computed with: exact Hamiltonian (continuous line); WH (diamonds); BDH with gauge 1 (circles); BDH with gauge 2 (cross); BDH with gauge 3 (squares).

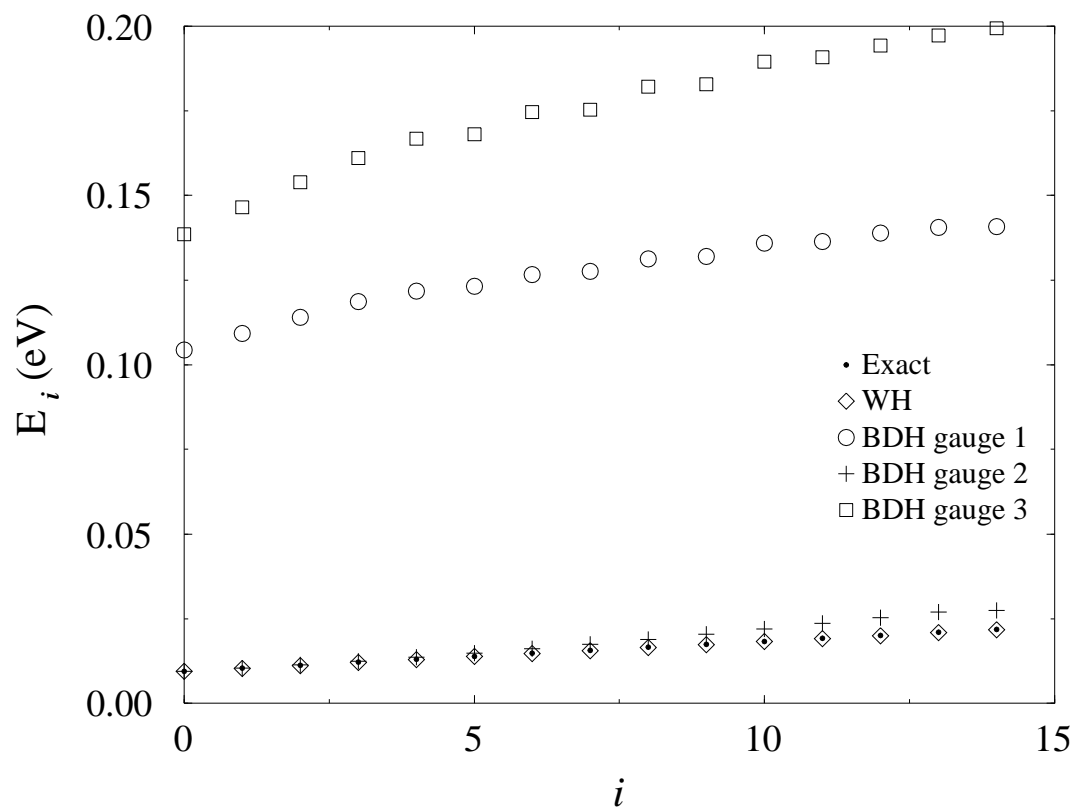
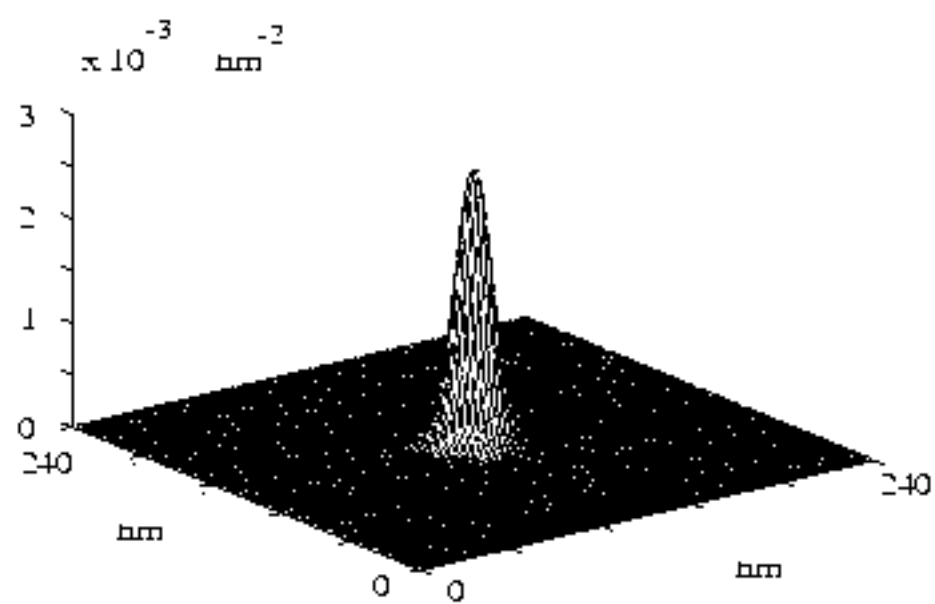


Fig . 1
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z) Exact



b) BDH gzuge 1

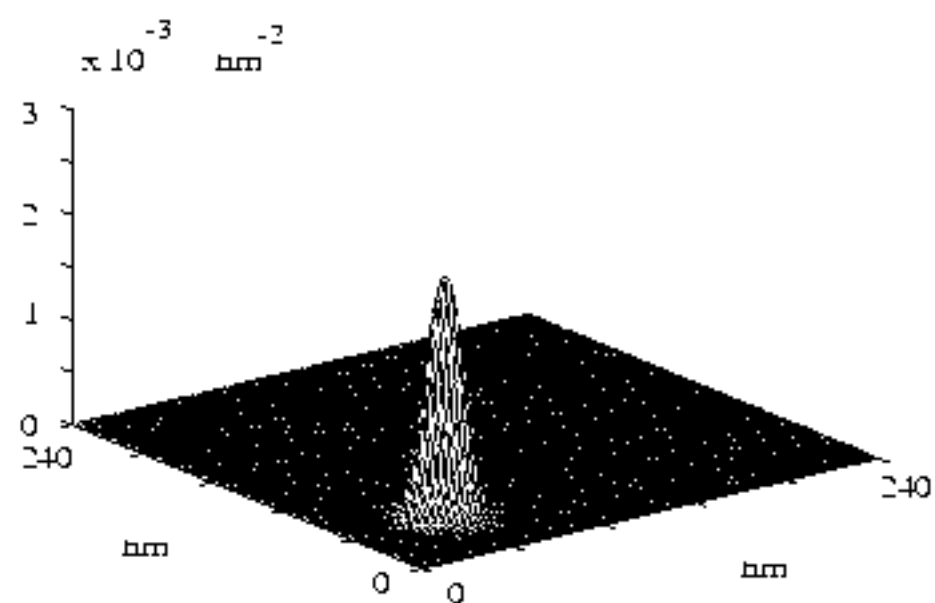
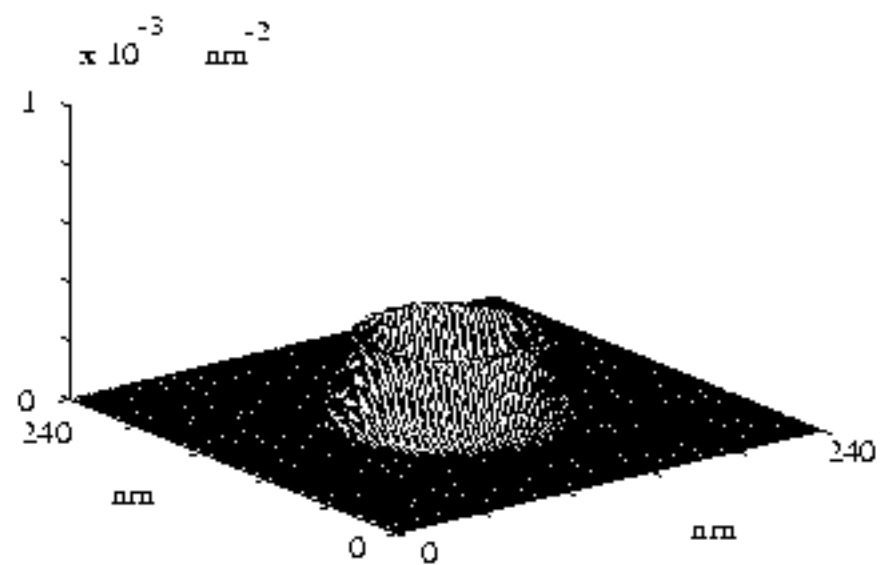


Fig. 2
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a) Exact



b) BDH gauge 2

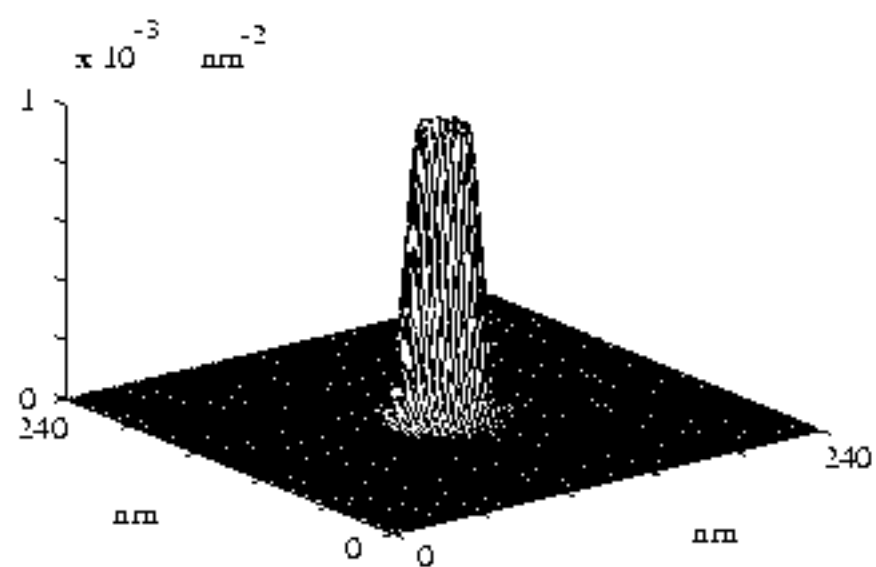


Fig. 3
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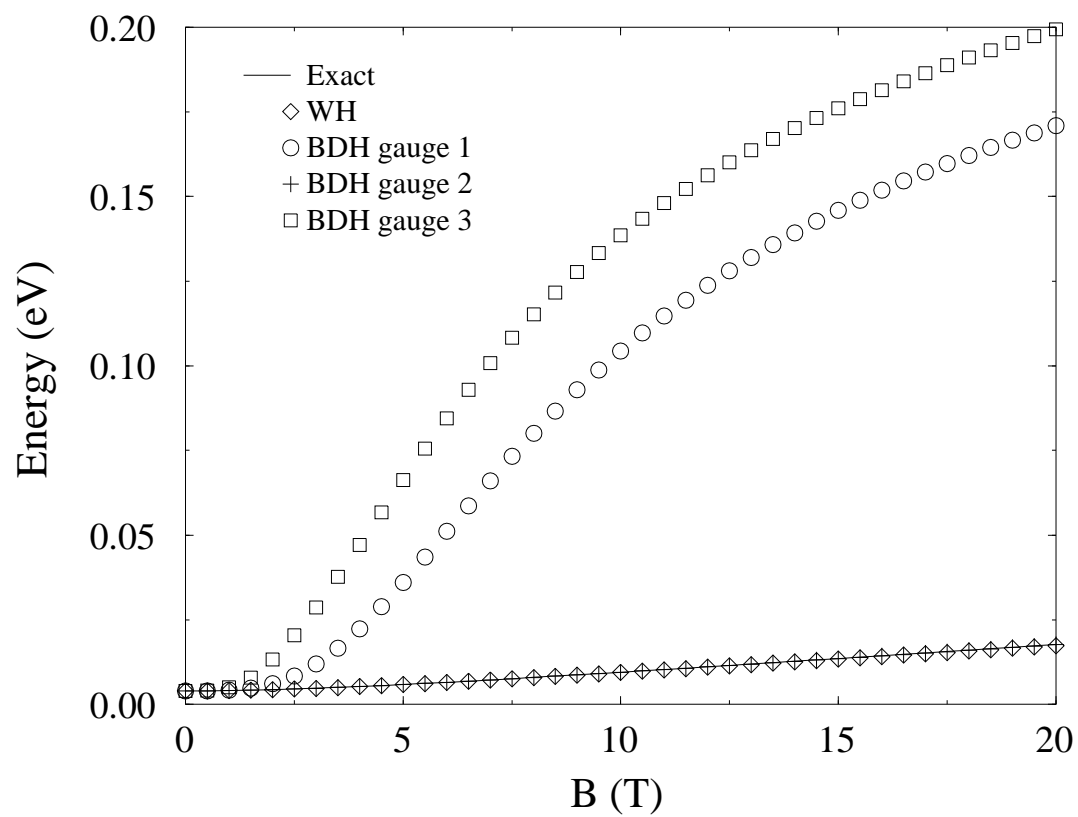


Fig. 4
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